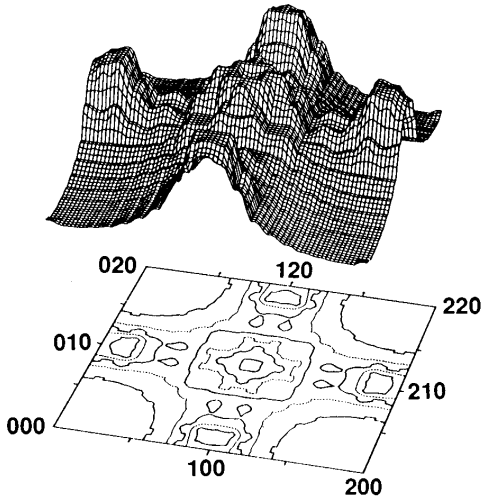
Theory, Modeling, and Computation

Advanced modeling techniques to solve real-world materials problems

Guided by fundamental theoretical principles and experimental procedures, we have developed a powerful computational technology to predict materials behavior. Computational technology provides a formidable arsenal for attacking problems in materials science and often alleviates the need for expensive experiments.

We divide materials classes into three categories, according to the degree with which we can gain a predictive understanding of materials behavior from the results of calculations based on quantum mechanics. Those categories are:

- Properties directly comparable to experimental findings. (Properties related to spectroscopy and electronic transport are often in this category.)
- Properties studied through phenomenological models. (The study of phase stability of alloys and compounds is in this category.)
- Properties not understandable within microscopic, quantum mechanical models. (Tribology and many mechanical properties such as superplasticity are in this category.)



Calculated x-ray diffuse scattering spectrum for an fcc-based $Cu_{80}Zn_{20}$ alloy.

APPLICATIONS

- *Electrostatics in electronic structure calculations*
- *Solid-state physics of actinide metals and their alloys*
- *Electromigration in metals and integrated circuits*
- *Mechanical properties of intermetallics*
- *Interpretation of positron annihilation spectroscopy and determination of Fermi surfaces*
- *Effects of defects and impurities at surfaces and interfaces*

Sample activities

- **Spectroscopy.** We use spin-polarized, angle-resolved photoemission spectroscopy to study nonmagnetic and magnetic crystalline surfaces. Our codes can handle various surface spectroscopies for the study of ordered surfaces with and without spin analysis.
- **Alloy phase stability.** Chemically disordered materials tend to order in particular configurations as functions of concentration, temperature, and pressure that affect the materials properties of substitutional alloys. We calculate alloy phase diagrams and related information on stability trends to bring important information to the alloy designer.
- **Molecular dynamics simulations.** We developed molecular dynamics codes that allow us to study processes such as ion implantation of dopants in silicon. Information generated by these codes, for example, helps us make physical predictions of dopant diffusion during rapid thermal annealing—a critical step in the processing of semiconductors.

Availability: Our modeling codes and expertise are available now. We seek industrial partners with whom we can develop modeling applications to solve real problems.

Contact

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